# Strong coupling expansion in a correlated three-dimensional topological insulator

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Motivated by recent studies which show that topological phases may emerge in strongly correlated electron systems, we theoretically study the strong electron correlation effect in a three-dimensional (3D) topological insulator, which effective Hamiltonian can be described by the Wilson fermion. We adopt $1/r$ long-range Coulomb interaction as the interaction between the bulk electrons. Based on the U(1) lattice gauge theory, the strong coupling expansion is applied by assuming that the effective interaction is strong. It is shown that the topological insulator phase changes to the normal insulator phase in the strong coupling limit, namely the value of the chiral condensate is not zero as well as in the case of graphene.

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## I. INTRODUCTION

Recently discovered topologically nontrivial phases have attracted many researchers and offered a new direction to modern physics[1,2]. Topologically nontrivial phase and trivial phase, in the presence of time-reversal symmetry, are distinguished by the $Z_2$ invariant[3,4]. Strong spin-orbit coupling is known to be essential to realize topological phases, since topological phases originate in the parity change in the lowest unoccupied band from even to odd induced by spin-orbit coupling. Topological phases are characterized by the gapless edge (surface) states which are protected by time-reveral symmetry. In 3D topological insulators, the surface states are described by the two-component massless Dirac fermions. The bulk states in such as $Bi_2Se_3$ are described by the four-component anisotropic massive Dirac fermions[5]. It is known that the surface states are robust against perturbation and disorder[6,7]. What about against electron correlation, i.e. Coulomb interaction? This is a natural question, because it has been revealed that strong electron correlation is important in many systems and may induce novel phenomena.

A novel Mott-insulating phase was found recently in an iridate[8], a $5d$-electron system, and has gathered much attention. Remarkably, the phase is induced by the cooperation of strong spin-orbit coupling and strong electron correlation. Evolved by this discovery, many studies have been done intensively in systems where both spin-orbit coupling and electron correlation exist, for the search for novel phases induced by them. Especially, it is of interest that topological phases such as the quantum spin Hall insulator[9] and the Weyl semimetal[10] are predicted in iridates. These results suggest that topological phases may emerge in strongly correlated $d$-electron systems. Preceding studies mainly focus on the competition between the spin or charge ordered phase and the topological phase in Hubbard-like models on honeycomb lattices[11–19], other 2D lattices[20–24] and 3D lattices[25–28]. Another study on the surface Dirac fermions shows that the Dirac fermions become massive with finite correlation strength due to the spotaneous magnetization[29].

On the other hand, the electron correlation effect in graphene, a two-dimensional Dirac fermion system, has been studied widely. In graphene in vacuum, the coupling constant becomes effectively large due to the small Fermi velocity. It has been predicted that a finite band gap is induced in charge neutral graphene in vacuum. In such a case, the strong coupling lattice gauge theory is applied[30–38]. The chiral condensate is the order parameter for the insulator-semimetal transition in the lattice gauge theory. It is noteworthy that lattice Monte Carlo studies show quantitatively correct critical value of the coupling strength below which the system becomes gapless[31,32,38] (graphene on a $SiO_2$ substrate is conducting). These results motivated us to do this study.

In this paper, we focus on the strong electron correlation effect in a 3D Dirac fermion system on a lattice which is a simple model describing a topologically nontrivial state. We adopt $1/r$ long-range Coulomb interaction as an interaction between the bulk electrons, because the screening effect in Dirac fermion systems is considered to be weak due to the vanishing of the density of states. This situation is nothing but what is described by the U(1) lattice gauge theory. Therefore, we can perform the strong coupling expansion of the lattice gauge theory by assuming that the effective coupling constant is large. The procedure is as follows. First we derive the effective action by the strong couling expansion. Next we calculate the effective potential (the free energy per unit volume at zero temperature) with the use of the Hubbard-Stratonovich transformation and the mean-field approximation. Finally we obtain the value of the chiral condensate as the stationary point of the effective potential.

The main purpose of this study is devided into three parts: (I) obtain the value of the chiral condensate, which corresponds to the excitation energy of the system, in the strong coupling limit. (II) search for the existence of the gapless (semimetal) phase between the topological and normal insulator phases. This is due to the fact that the transition from topologically nontrivial phase to trivial phase (and vice versa) needs the gap closing of the bulk energy band. (III) search for the phase in

which time-reversal and inversion symmetries are spontaneously broken due to electron correlation. Such a phase has been confirmed in the lattice quantum chromodynamics (QCD) with Wilson fermions[39–41] and was suggested recently in a mean-field study of Wilson fermions with the short-range interaction[42].

## II. MODEL

It is known that the effective Hamiltonian of 3D topological insulators such as $Bi_2Se_3$ is described by the Wilson fermion[5]:

$$\mathcal{H}_0(\boldsymbol{k}) = \sum\nolimits_j \sin k_j \cdot \alpha_j + m(\boldsymbol{k})\beta, \tag{1}$$

where $m(\boldsymbol{k}) = m_0 + r\sum_j (1-\cos k_j)$, $r > 0$, $j\ (=1,2,3)$ denotes spacial axis, and $\alpha_j$, $\beta$ are the Dirac gamma matrices given by

$$\alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}, \qquad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{2}$$

The energy of this system is measured in units of $v_{\mathrm{F}}/a$ with $v_{\mathrm{F}}$ and $a$ being the Fermi velocity and the lattice constant, respectively. The Hamiltonian (1) has time-reversal ($\mathcal{T}$) symmetry and inversion ($\mathcal{I}$) symmetry, i.e., $\mathcal{T}\mathcal{H}_0(\boldsymbol{k})\mathcal{T}^{-1} = \mathcal{H}_0(-\boldsymbol{k})$ and $\mathcal{I}\mathcal{H}_0(\boldsymbol{k})\mathcal{I}^{-1} = \mathcal{H}_0(-\boldsymbol{k})$ are satisfied, where $\mathcal{T} = \mathbf{1}\otimes(-i\sigma_2)\mathcal{K}$ ($\mathcal{K}$ is the complex conjugation operator) and $\mathcal{I} = \sigma_3 \otimes \mathbf{1}$. In the Hamiltonian (1), the spinor is written in the basis of $\left[c^\dagger_{\boldsymbol{k}A\uparrow}, c^\dagger_{\boldsymbol{k}A\downarrow}, c^\dagger_{\boldsymbol{k}B\uparrow}, c^\dagger_{\boldsymbol{k}B\downarrow}\right]$, where $c^\dagger$ is the creation operator of an electron, $A$, $B$ denote two orbitals, and $\uparrow$ ($\downarrow$) denotes up- (down-) spin[5].

In the presence of time-reversal symmetry and inversion symmetry, the $Z_2$ invariant of the system is given by[3,4]

$$(-1)^\nu = \prod_{i=1}^{8} \left\{-\mathrm{sgn}\left[m\left(\boldsymbol{\Lambda}_i\right)\right]\right\}, \tag{3}$$

where $\boldsymbol{\Lambda}_i$ are the eight time-reversal invariant momenta. It is easily shown that if $0 > m_0 > -2r$ or $-4r > m_0 > -6r$ ($m_0 > 0$, $-2r > m_0 > -4r$, or $-6r > m_0$), the system is topologically nontrivial (trivial).

Let us consider a strongly correlated topological insulator in Euclidean spacetime, which is described by the Wilson fermion with $1/r$ Coulomb interaction between the bulk electrons. We start from the Euclidean action of (3+1)D Wilson fermion interacting with electromagnetic field on a lattice, which is given by

$$\begin{aligned} S_F = &-\sum_{n,\mu}\left[\bar{\psi}_n P^-_\mu U_{n,\mu}\psi_{n+\hat{\mu}} + \bar{\psi}_{n+\hat{\mu}} P^+_\mu U^\dagger_{n,\mu}\psi_n\right] \\ &+ (m_0+4r)\sum_n \bar{\psi}_n\psi_n, \end{aligned} \tag{4}$$

where $P^\pm_\mu = (r \pm \gamma_\mu)/2$. Here $n = (n_0, n_1, n_2, n_3)$ denotes a site on a spacetime lattice and $\hat{\mu}$ ($\mu = 0,1,2,3$) denotes the unit vector along $\mu$-direction. $U_{n,\mu}$ is the link variable, which is defined by $U_{n,\mu} = e^{iagA_\mu(n+\hat{\mu}/2)}$, where $A_\mu = (A_0, \boldsymbol{A})$ is the four-vector potential, $a$ is the lattice constant, and $g^2 = e^2/\epsilon$ with $e$ and $\epsilon$ being electric charge and the permittivity of the system, respectively. The term proportional to $r$ is introduced to eliminate fermion doublers. In this paper, according to the Hamiltonian (1), we adopt the Dirac representation in the Euclidean spacetime ($\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$):

$$\gamma_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \gamma_j = \begin{bmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{bmatrix}, \quad \gamma_5 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{5}$$

where $j = 1,2,3$ and $\sigma_j$ are the Pauli matrices.

In the case of 3D topological insulators, the Fermi velocity $v_{\mathrm{F}}$ is about $3\times10^{-3}c$ where $c$ is the speed of light in vacuum. Then the interactions between the bulk electrons can be regarded as only the instantaneous Coulomb interaction ($A_j = 0$) like in the case of graphene[30–38], so the action (4) is rewritten as

$$S_F = S_F^{(\tau)} + S_F^{(s)} + (m_0+4r)\sum_n \bar{\psi}_n\psi_n, \tag{6}$$

where

$$\begin{cases} S_F^{(\tau)} = -\displaystyle\sum_n\left[\bar{\psi}_n P^-_0 U_{n,0}\psi_{n+\hat{0}} + \bar{\psi}_{n+\hat{0}} P^+_0 U^\dagger_{n,0}\psi_n\right] \\ S_F^{(s)} = -\displaystyle\sum_{n,j}\left[\bar{\psi}_n P^-_j \psi_{n+\hat{j}} + \bar{\psi}_{n+\hat{j}} P^+_j \psi_n\right], \end{cases} \tag{7}$$

and $U_{n,0} = e^{i\theta_n}$ ($-\pi \le \theta_n \le \pi$). The pure U(1) gauge action on a lattice is given by

$$S_G = \beta\sum_n\sum_{\mu>\nu}\left[1 - \frac{1}{2}\left(U_{n,\mu\nu} + U^\dagger_{n,\mu\nu}\right)\right], \tag{8}$$

where $\beta = v_{\mathrm{F}}/g^2$. The plaquette contribution $U_{n,\mu\nu}$ is defined by

$$U_{n,\mu\nu} = U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu}, \tag{9}$$

where $U_{n,j} = 1$ in our case. The total action on a lattice is written as

$$S = S_F + S_G. \tag{10}$$

The dielectric constant $\epsilon_r$ of $Bi_2Se_3$ is rather large[43] ($\epsilon_r = \epsilon/\epsilon_0 \approx 100$). This means that the Coulomb interaction between the bulk electrons in $Bi_2Se_3$ is considered to be weak. In fact, the value of $\beta$ is approximated as

$$\beta = \frac{v_{\mathrm{F}}\epsilon_r}{4\pi c}\cdot\frac{4\pi\epsilon_0\hbar c}{e^2} \approx 3, \tag{11}$$

and we cannot perform the strong coupling expansion in $Bi_2Se_3$. However, we think it would be important from a theorerical viewpoint to examine the strong electron correlation effect in Dirac fermion systems which describe topologically nontrivial states.

## III. EFFECTIVE ACTION

Let us perform the strong coupling expansion. The strong coupling expansion has been often used in QCD[44–48] where the coupling between fermions (quarks) and gauge fields (gluons) are strong. We can carry out the $U_0$ integral by using the SU($N_c$) group integral formulae:

$$\int dU 1 = 1, \quad \int dU U_{ab} = 0, \quad \int dU U_{ab} U^{\dagger}_{cd} = \frac{1}{N_c}\delta_{ad}\delta_{bc}. \tag{12}$$

In the following, we derive the effective action $S_{\text{eff}}[\psi, \bar{\psi}]$ by carrying out the $U_0$ integral:

$$Z = \int \mathcal{D}[\psi, \bar{\psi}, U_0] e^{-S_F - S_G} = \int \mathcal{D}[\psi, \bar{\psi}] e^{-S_{\text{eff}}}. \tag{13}$$

First we consider the strong coupling limit ($\beta = 0$). In this case, the timelike partition function is given by

$$Z^{(\tau)}_{\text{SCL}}[\psi, \bar{\psi}] = \int \mathcal{D}U_0 e^{-S^{(\tau)}_F}. \tag{14}$$

Integration with respect to $U_0$ is carried out to be

$$Z^{(\tau)}_{\text{SCL}} = \exp\left[\sum_n \bar{\psi}_n P^-_0 \psi_{n+\hat{0}} \bar{\psi}_{n+\hat{0}} P^+_0 \psi_n\right]. \tag{15}$$

Here we have used the fact that the grassmann variables $\psi$'s and $\bar{\psi}$'s satisfy $\psi^2 = \bar{\psi}^2 = 0$. We can rewrite this term as

$$\bar{\psi}_n P^-_0 \psi_{n+\hat{0}} \bar{\psi}_{n+\hat{0}} P^+_0 \psi_n = -\text{tr}\left[M_n P^+_0 M_{n+\hat{0}} P^-_0\right], \tag{16}$$

where we have defined $(M_n)_{\alpha\beta} = \bar{\psi}_{n,\alpha}\psi_{n,\beta}$. The subscripts $\alpha$ and $\beta$ denote the component of spinors.

Next we evaluate the term of the order of $\beta$. In order to evaluate the plaquette contributions from $S_G$, we use the cumulant expansion[48,49]. Let us define an expectation value:

$$\langle A \rangle \equiv \frac{1}{Z^{(\tau)}_{\text{SCL}}} \int \mathcal{D}U_0 A[U_0] e^{-S^{(\tau)}_F}. \tag{17}$$

Then using this definition, the full timelike partition function can be expressed as

$$Z^{(\tau)} = \int \mathcal{D}U_0 e^{-S^{(\tau)}_F - S_G} = Z^{(\tau)}_{\text{SCL}} \left\langle e^{-S_G} \right\rangle. \tag{18}$$

The contribution from $S_G$ is given by

$$\Delta S \equiv -\log\left\langle e^{-S_G}\right\rangle = -\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left\langle S^n_G \right\rangle_c, \tag{19}$$

where $\langle \cdots \rangle_c$ is a cumulant. The correction to the action up to $\mathcal{O}(\beta)$ is given by

$$\begin{aligned} \Delta S &= \langle S_G \rangle_c = \langle S_G \rangle \\ &= -\frac{\beta}{2} \sum_n \sum_{\mu>\nu} \left\langle U_{n,\mu\nu} + U^{\dagger}_{n,\mu\nu} \right\rangle. \end{aligned} \tag{20}$$

The expectation value of $U_{n,\mu\nu}$ is evaluated as follows[48]:

$$\langle U_{n,\mu\nu} \rangle \simeq \int dU_{n,0} U_{n,\mu\nu} e^{-s^{(\tau)}_P}, \tag{21}$$

where $s^{(\tau)}_P$ is the plaquette-related part of $S^{(\tau)}_F$. We see that the terms with $(\mu,\nu) = (i,j)$ become constant and find only $(\mu,\nu) = (j,0)$ terms to survive:

$$\begin{cases} \langle U_{n,j0} \rangle = -\text{tr}\left[V^+_{n,j} P^+_0 V^-_{n+\hat{0},j} P^-_0\right], \\ \left\langle U^{\dagger}_{n,j0} \right\rangle = -\text{tr}\left[V^-_{n,j} P^+_0 V^+_{n+\hat{0},j} P^-_0\right], \end{cases} \tag{22}$$

where we have defined $\left(V^+_{n,j}\right)_{\alpha\beta} = \bar{\psi}_{n,\alpha}\psi_{n+\hat{j},\beta}$ and $\left(V^-_{n,j}\right)_{\alpha\beta} = \bar{\psi}_{n+\hat{j},\alpha}\psi_{n,\beta}$.

Finally, substituting Eqs. (15) and (20) to Eq. (18), we obtain the effective action up to $\mathcal{O}(\beta)$:

$$\begin{aligned} S_{\text{eff}} =& (m_0 + 4r)\sum_n \bar{\psi}_n \psi_n - \sum_{n,j}\left[\bar{\psi}_n P^-_j \psi_{n+\hat{j}} + \bar{\psi}_{n+\hat{j}} P^+_j \psi_n\right] \\ &+ \sum_n \text{tr}\left[M_n P^+_0 M_{n+\hat{0}} P^-_0\right] \\ &+ \frac{\beta}{2}\sum_{n,j}\left\{\text{tr}\left[V^+_{n,j} P^+_0 V^-_{n+\hat{0},j} P^-_0\right] + (V^+ \longleftrightarrow V^-)\right\}. \end{aligned} \tag{23}$$

## IV. EFFECTIVE POTENTIAL AND CHIRAL CONDENSATE

In this section, we derive the effective potential with the use of the extended Hubbard-Stratonovich transformation (EHS)[35–37,48], and then we obtain the value of the chiral condensate as the stationary point of the effective potential. We apply the EHS to the trace of arbitrary two matrices. Introducing two auxiliary fields $R$ and $R'$, we obtain

$$\begin{aligned} & e^{\kappa \text{tr} AB} \propto \\ & \int \mathcal{D}[R, R'] \exp\left\{-\kappa \sum_{\alpha\beta}\left[(R_{\alpha\beta})^2 + (R'_{\alpha\beta})^2\right.\right. \\ & \left.\left. -(A_{\alpha\beta} + B^T_{\alpha\beta})R_{\beta\alpha} - i(A_{\alpha\beta} - B^T_{\alpha\beta})R'_{\beta\alpha}\right]\right\}, \end{aligned} \tag{24}$$

where $\kappa$ is a positive constant and the superscript $T$ denotes the transpose of a matrix. Two auxiliary fields take the saddle point value, $R_{\alpha\beta} = \left\langle A + B^T \right\rangle_{\beta\alpha}$ and $R'_{\alpha\beta} = i\left\langle A - B^T \right\rangle_{\beta\alpha}$, respectively. Defining $Q = R + iR'$, Eq. (24) is rewritten as

$$\begin{aligned} & e^{\kappa \text{tr} AB} \propto \\ & \int \mathcal{D}[Q, Q^*] \exp\left\{-\kappa \sum_{\alpha\beta}\left[|Q_{\alpha\beta}|^2 - A_{\alpha\beta}Q_{\beta\alpha} - B^T_{\alpha\beta}Q^*_{\beta\alpha}\right]\right\}. \end{aligned} \tag{25}$$

### A. Effective Potential in the Strong Coupling Limit

We consider to decouple the third term in the effective action (23) to fermion bilinear form. To do this, we set $(\kappa, A, B) = (1, M_n P_0^+, -M_{n+\hat{0}} P_0^-)$ in Eq. (25). Assuming that $Q^\dagger = Q$ ($Q^*_{\beta\alpha} = Q_{\alpha\beta}$) and performing the mean-field approximation, $Q_{n-\hat{0}} = Q_n = \text{const.}$, we obtain

$$\begin{aligned} &\exp\left\{-\sum_n \mathrm{tr}\left[M_n P_0^+ M_{n+\hat{0}} P_0^-\right]\right\} \\ &\propto \int \mathcal{D}Q \exp\left\{-\sum_n \left[\left|(Q_n)_{\alpha\beta}\right|^2 - \bar{\psi}_n \left(\gamma_0 Q\right)^T \psi_n\right]\right\}, \end{aligned} \tag{26}$$

where we have used that $[M_n \gamma_0]_{\alpha\beta} = \bar{\psi}_{n,\alpha}\psi_{n,\gamma}(\gamma_0)_{\gamma\beta}$. In this case, $Q$ has the saddle point value

$$\begin{aligned} Q_{\alpha\beta} &= \frac{1}{2}\left\langle \left[M_n P_0^+\right] - \left[M_n P_0^-\right]\right\rangle_{\beta\alpha} \\ &= \frac{1}{2}\left\langle M_n \gamma_0\right\rangle_{\beta\alpha}. \end{aligned} \tag{27}$$

We obtain the effective action in the strong coupling limit expressed by an complex auxiliary field $Q$:

$$Z = \int \mathcal{D}[\psi, \bar{\psi}, Q] e^{-S_{\mathrm{eff}}[\psi,\bar{\psi},Q]}, \tag{28}$$

where

$$S_{\mathrm{eff}} = N_s N_\tau \sum_{\alpha,\beta} |Q_{\alpha\beta}|^2 + \sum_k \bar{\psi}_k \mathcal{M}(\boldsymbol{k}, Q)\psi_k \tag{29}$$

with

$$\begin{aligned} \mathcal{M} =& \sum_j i\gamma_j \sin k_j + \left[m_0 + r\left(4 - \sum_j \cos k_j\right)\right] I \\ &- \left(\gamma_0 Q\right)^T. \end{aligned} \tag{30}$$

Here $N_s = V/a^3$ and $N_\tau = 1/T$ with $V$ and $T$ being the volume and the temperature of the system, respectively and we have done Fourier transform from $n = (n_0, n_1, n_2, n_3)$ to $k = (k_0, k_1, k_2, k_3)$.

The effective potential at zero temperature per unit spacetime volume is given by

$$\mathcal{F}_{\mathrm{eff}}[Q] = -\frac{1}{N_s N_\tau} \log Z[Q]. \tag{31}$$

Integration with respect to $\psi$ and $\bar{\psi}$ is carried out by the formula $\int D[\psi, \bar{\psi}] e^{-\bar{\psi}\mathcal{M}\psi} = \det\mathcal{M}$. Therefore we need to calculate the determinant of $\mathcal{M}$. Here let us assume that

$$\begin{aligned} \langle M_n \rangle &= \sigma e^{i\theta\gamma_5} = \sigma(\cos\theta I + i\sin\theta\gamma_5) \\ &= \sigma \begin{bmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{bmatrix}. \end{aligned} \tag{32}$$

Then it follows that

$$\begin{cases} \left\langle \bar{\psi}\psi \right\rangle = \sigma\cos\theta \equiv \phi_\sigma \\ \left\langle \bar{\psi} i\gamma_5 \psi \right\rangle = \sigma\sin\theta \equiv \phi_\pi. \end{cases} \tag{33}$$

The terms $\left\langle \bar{\psi}\psi \right\rangle$ and $\left\langle \bar{\psi} i\gamma_5 \psi \right\rangle$ decribe the chiral condensate and the condensate of pseudoscalar mode, respectively. The Wilson fermion breaks the chiral symmetry by itself (the term proportional to $r$), hence we use the value of $\left\langle \bar{\psi}\psi \right\rangle$ to determine the system is whether insulating or semimetallic. Namely, if $\left\langle \bar{\psi}\psi \right\rangle \neq 0$, the mass gap is dynamically generated and thus the system is insulating.

From Eqs. (27), (30) and (32), we obtain

$$\begin{aligned} \mathcal{M} &= \begin{bmatrix} m_{\boldsymbol{k}} - \frac{1}{2}\phi_\sigma & \sigma_j \sin k_j - i\frac{1}{2}\phi_\pi \\ -\sigma_j \sin k_j - i\frac{1}{2}\phi_\pi & m_{\boldsymbol{k}} - \frac{1}{2}\phi_\sigma \end{bmatrix} \\ &\equiv \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \end{aligned} \tag{34}$$

where we have defined that $m_{\boldsymbol{k}} = m_0 + r\left(4 - \sum_j \cos k_j\right)$. After a straightforward calculation, we have

$$\begin{aligned} \det\mathcal{M} &= \det A \cdot \det\left(D - CA^{-1}B\right) \\ &= \left[\sum_j \sin^2 k_j + \left(m_{\boldsymbol{k}} - \frac{\phi_\sigma}{2}\right)^2 + \left(\frac{\phi_\pi}{2}\right)^2\right]^2. \end{aligned} \tag{35}$$

Finally we arrive at the effective potential in the strong coupling limit:

$$\begin{aligned} \mathcal{F}_{\mathrm{eff}}(\phi_\sigma, \phi_\pi) &= \phi_\sigma^2 + \phi_\pi^2 - 2\int_{-\pi}^{\pi} \frac{d^3k}{(2\pi)^3} \\ &\times \log\left[\sum_j \sin^2 k_j + \left(m_{\boldsymbol{k}} - \frac{\phi_\sigma}{2}\right)^2 + \left(\frac{\phi_\pi}{2}\right)^2\right]. \end{aligned} \tag{36}$$

The values of $\phi_\sigma$ and $\phi_\pi$ are obtained by the stationary conditions $\partial\mathcal{F}_{\mathrm{eff}}(\phi_\sigma, \phi_\pi)/\partial\phi_\sigma = \partial\mathcal{F}_{\mathrm{eff}}(\phi_\sigma, \phi_\pi)/\partial\phi_\pi = 0$.

In the chiral limit ($r = m_0 = 0$), the effective potential is a function of only $\sigma$, reflecting the chiral symmetry of the action. Note that this effective potential corresponds to that of the staggered fermion (SF) model for graphene[35,36] except for an additional factor 4 by setting $r = 0$ and changing from (3+1)D to (2+1)D:

$$\mathcal{F}_{\mathrm{eff}}(\phi_\sigma, \phi_\pi) = 4\mathcal{F}^{\mathrm{SF}}_{\mathrm{eff}}(\phi_\sigma, \phi_\pi). \tag{37}$$

This result is reasonable, because the two cases describes the same system where the $2^3 = 8$ fermion doublers appear.

### B. Chiral Condensate in the Strong Coupling Limit

At first, we found that the value of $\phi_\pi$ is zero at the stationary point for any set of $(r, m_0)$. Hence in the following, we set $\phi_\sigma = -\sigma$ and $\phi_\pi = 0$ in Eq. (36) to calculate the value of the chiral condensate $\sigma$. The term $i\bar{\psi}\gamma_5\psi$ is odd under both time-reversal and inversion. Therefore, this means that the phase with spontaneously broken time-reversal and inversion symmetries does not arise in the strong coupling (electron correlation) limit.

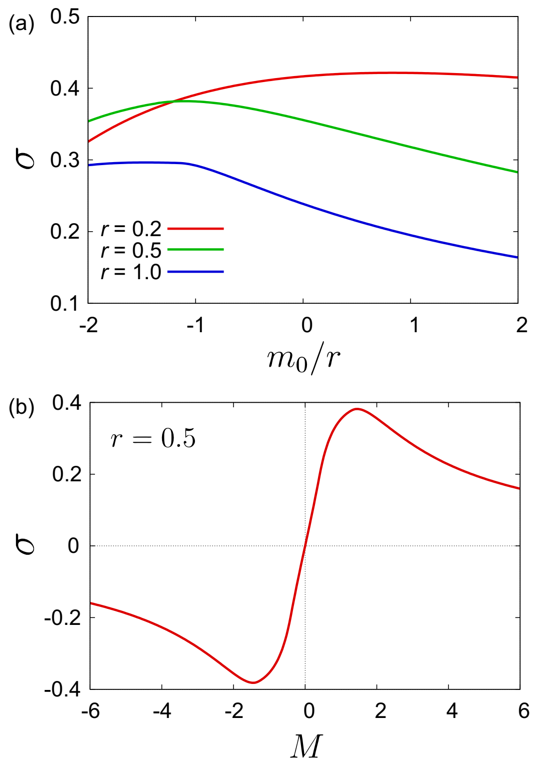


FIG. 1. (Color online) (a) $m_0$-dependence and (b) $M$-dependence of the chiral condensate $\sigma$ in the strong coupling limit ($\beta = 0$). We define $M = m_0 + 4r$.

A mean-field study of Wilson fermions with the short-range interaction from the weak coupling[42] suggests the existence of this phase. Such a phase (where parity and flavor symmetry are spotaneously broken) has also confirmed in the lattice QCD with Wilson fermions[39–41].

The $m_0$- and $M$-dependence of the chiral condensate $\sigma$ is shown in Fig. 1. Here we define $M = m_0 + 4r$. The value of $\sigma$ is expected to be quantitatively correct, based on the fact that the result of a strong coupling expansion study in graphene[35,36] is in good agreement with that of lattice Monte Carlo studies[30–33]. As mentioned above, at $\beta = \infty$ (i.e. non-interacting limit), the system with $0 > m_0 > -2r$ ($m_0 > 0$) is identified as a topological (normal) insulator. The chiral condensate is dynamically generated mass gap and corresponds to the excitation energy of the system. Therefore, the topological insulator phase changes to the normal insulator phase in the strong coupling limit. This is consistent with a mean-field analysis from the weak coupling[42]. The value of the energy gap in the strong coupling limit is estimated as $\sigma/2 \cdot \hbar v_{\mathrm{F}}/a \simeq 0.14$ [eV] at $(r, m_0) = (1.0, -0.5)$, when $\hbar v_{\mathrm{F}} = 3$ [eV·Å] and $a = 3$ [Å] are assumed. From Fig. 1(b), we see that $\sigma$ approaches zero as $M$ approaches zero and that $\sigma$ gets proportional to $1/M$ as $r$ becomes larger. This $r$-dependence is similar to that in the lattice QCD with Wilson fermions[39], which is given by

$$\sigma = \begin{cases} \dfrac{1}{M} & (|M| > 2) \\ \dfrac{3M}{16 - M^2} & (|M| < 2). \end{cases} \tag{38}$$

However, in the region near $|M| = 2$, $\sigma$ is a smooth function of $M$ in contrast to Eq. (38).

### C. Effective Potential Up to $\mathcal{O}(\beta)$

Let us evaluate the $\mathcal{O}(\beta)$ contribution to the effective potential. We write the fourth term in the effective action (23) as $\Delta S_1 + \Delta S_2$. Then we should choose such that $(\kappa, A, B) = (\beta/2, V^+_{n,j} P^+_0, -V^-_{n+0,j} P^-_0)$ in Eq. (24):

$$\begin{aligned} e^{-\Delta S_1} \propto \exp\Bigg\{ -\frac{\beta}{2} \sum_j \Bigg[ & \sum_n \left[ (R^j_{\alpha\beta})^2 + (T^j_{\alpha\beta})^2 \right] \\ & - \sum_k \bar{\psi}_k \Big[ \left( e^{ik_j} R^{jT} P^+_0 - e^{-ik_j} R^j P^-_0 \right) \\ & - i \left( e^{ik_j} T^{jT} P^+_0 + e^{-ik_j} T^j P^-_0 \right) \Big] \psi_k \Bigg] \Bigg\}. \end{aligned} \tag{39}$$

Similarly, setting $(\kappa, A, B) = (\beta/2, V^-_{n,j} P^+_0, -V^+_{n+0,j} P^-_0)$, we obtain

$$\begin{aligned} e^{-\Delta S_2} \propto \exp\Bigg\{ -\frac{\beta}{2} \sum_j \Bigg[ & \sum_n \left[ (R'^j_{\alpha\beta})^2 + (T'^j_{\alpha\beta})^2 \right] \\ & - \sum_k \bar{\psi}_k \Big[ \left( e^{-ik_j} R'^{jT} P^+_0 - e^{ik_j} R'^j P^-_0 \right) \\ & - i \left( e^{-ik_j} T'^{jT} P^+_0 + e^{ik_j} T'^j P^-_0 \right) \Big] \psi_k \Bigg] \Bigg\}. \end{aligned} \tag{40}$$

These two equations are very complicated. It is natural to suppose the following two cases:

$$\begin{cases} \text{(i) } R = R' \text{ and } T = T' \\ \text{(ii) } R = -R' \text{ and } T = -T'. \end{cases} \tag{41}$$

It is shown that the effective potential of the case (ii) is smaller than that of the case (i) [see Appendix]. Thus we show the calculation in the case (ii) in the following. In this case, combining Eqs. (39) and (40), we have

$$\begin{aligned} \Delta S[\psi, \bar{\psi}, R, T] = \beta \sum_j \Bigg\{ & \sum_n \left[ (R^j_{\alpha\beta})^2 + (T^j_{\alpha\beta})^2 \right] \\ & + \sum_k \bar{\psi}_k \Big[ -i \left( R^{jT} P^+_0 + R^j P^-_0 \right) \\ & + T^{jT} P^+_0 - T^j P^-_0 \Big] \sin k_j \psi_k \Bigg\}. \end{aligned} \tag{42}$$

It have been found in the previous subsection that the value of $\langle\bar{\psi}i\gamma_5\psi\rangle$, the condensate of pseudoscalar mode, is zero for any $M$ in the strong coupling limit. Hence, we concentrate on examining the $\beta$-dependence of the chiral condensate. For this purpose, we assume that Eq. (42) takes time-reversal and inversion symmetric form which results from the original Lagrangian. That is, we assume that $\left(R^{jT}P_0^+ + R^jP_0^-\right) = a\gamma_j$ and $\left(T^{jT}P_0^+ - T^jP_0^-\right) = b\gamma_j$ where $a$ and $b$ are constants, since $\sin k_j$ is odd under time-reversal.

To be concrete, we set as follows:

$$\begin{cases} R^j = \phi_j\gamma_j = \phi_j\begin{bmatrix} 0 & i\sigma_j \\ -i\sigma_j & 0 \end{bmatrix}, \\ T^j = i\omega_j\gamma_j\gamma_0 = \omega_j\begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}, \end{cases} \tag{43}$$

where $\phi_j$, $\omega_j$ are constants. It is easily found that $R^2$, $T^1$ and $T^3$ are symmetric, and that $R^1$, $R^3$ and $T^2$ are antisymmetric. However, the final result doesn't depend on whether the auxiliary field is symmetric or antisymmetric. Substituting Eq. (43) to Eq. (42), we see that the correction from the strong coupling limit is obtained by replacing $\sin k_j$ in $\mathcal{M}(\boldsymbol{k},\sigma)$ (Eq. (34)) by $(1-\beta r\phi_j+\beta\omega_j)\sin k_j$. This means that the effect of $\beta$ is equivalent to the modification the Fermi velocity from the strong coupling limit. Then we obtain the effective potential expressed by auxiliary fields:

$$\begin{aligned} \mathcal{F}_{\text{eff}}(\sigma,\phi_j,\omega_j) &= \sigma^2 + 4\beta\sum_j(\phi_j^2+\omega_j^2) \\ &- \int_{-\pi}^{\pi}\frac{d^3k}{(2\pi)^3}\log\left[\det\mathcal{M}(\boldsymbol{k},\sigma,\phi_j,\omega_j)\right]. \end{aligned} \tag{44}$$

Eliminating $\phi_j$ and $\omega_j$ by the stationary conditions $\partial F_{\text{eff}}(\sigma,\phi_j,\omega_j)/\partial\phi_j = \partial F_{\text{eff}}(\sigma,\phi_j,\omega_j)/\partial\omega_j = 0$, we arrive at the effective potential up to $\mathcal{O}(\beta)$:

$$\begin{aligned} \mathcal{F}_{\text{eff}}(\sigma) &= \sigma^2 - 2\int_{-\pi}^{\pi}\frac{d^3k}{(2\pi)^3}\log\left[\left(m_{\boldsymbol{k}}-\frac{\sigma}{2}\right)^2+\sum_l\sin^2 k_l\right] \\ &- (1+r^2)\beta\sum_{j=1}^{3}\left[\int_{-\pi}^{\pi}\frac{d^3k}{(2\pi)^3}\frac{\sin^2 k_j}{\left(m_{\boldsymbol{k}}-\frac{\sigma}{2}\right)^2+\sum_l\sin^2 k_l}\right]^2. \end{aligned} \tag{45}$$

As well as in the strong couling limit, this effective potential gives the same value of the chiral condensate as that of the staggered fermion (SF) model for graphene[35,36] by setting $r=0$ and changing from (3+1)D to (2+1)D: $\mathcal{F}_{\text{eff}}(\sigma) = 4\mathcal{F}_{\text{eff}}^{\text{SF}}(\sigma)$.

### D. $\beta$-dependence of Chiral Condensate

The $\beta$-dependence of the chiral condensate $\sigma$ is shown in Fig. 2. We see that $\sigma$ is a monotonically decreasing function of the coupling strength $\beta$. This behavior is consistent with a mean-field analysis from the weak coupling[42]. Our result shows that the mass gap remains finite, in contrast to the mean-field analysis in which the mass gap becomes infinity in the strong coupling limit. We see also that as $r$ becomes smaller, the rate of decrease of $\sigma$ becomes notable. Namely, as the original mass of doublers becomes smaller, the energy gap of the system becomes smaller, as is understood intuitively.

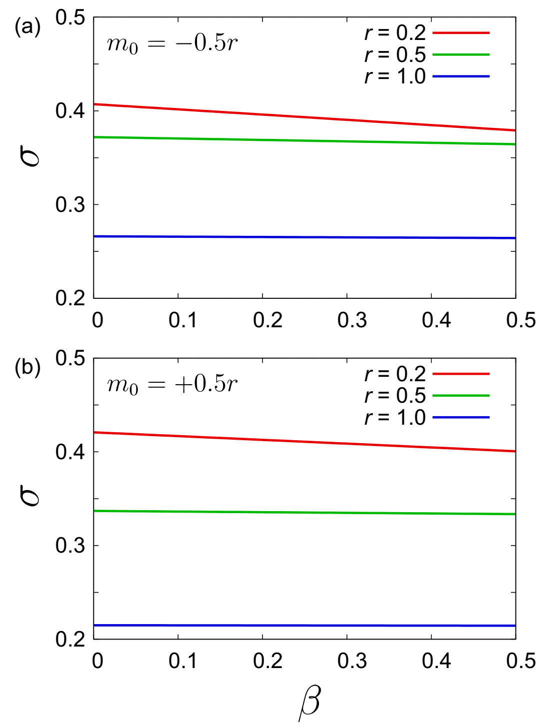


FIG. 2. (Color online) $\beta$-dependence of the chiral condensate $\sigma$ with (a) $m_0 = -0.5r$ and (b) $m_0 = +0.5r$.

It is concluded that the gapped phase (normal insulator phase) is stable in the strong coupling region. This contrasts with the result of the strong coupling expansion in graphene[35,36]. In graphene, the rate of decrease of $\sigma$ from $\beta=0$ to $\beta=0.5$ is about 60%[36], whereas that of our model is about 10% at $r=0.2$. The difference between these two cases stems from the spatial dimension (two and three). This is because the staggered fermion model for graphene and the $r=0$ limit of our model differ only by the dimension.

## V. SUMMARY

To summarize, we have studied the strong electron correlation effect in a 3D topological insulator which effective Hamiltonian can be described by the Wilson fermion. Based on the U(1) lattice gauge theory, we have performed the strong coupling expansion. We have found that the system always has a finite enery gap in the strong coupling region. The values of the chiral condensate which is regarded as the energy gap of the system in

the strong coupling limit are expected to be correct quantitatively. The behavior of the chiral condensate in our model is similar to that of the lattice QCD with Wilson fermions. The phase where time-reversal and inversion symmetries are spontaneously broken was not found in the strong coupling limit, in contrast to the case of the lattice QCD.

The critical value of coupling strength, at which the system changes from insulator to semimetal, could not be obtained, although it was shown that the energy gap becomes smaller as electron correlation gets weaker. For the consistency with the result in a weak coupling analysis, it is concluded that the topological insulator phase changes to the normal insulator phase in the strong coupling limit. In this study, the bulk property of a 3D topological insulator was examined. It will be interesting to examine the strong correlation effect in the surface Dirac fermions.

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### Appendix A: Determination of Effective Potential

In this appendix, we show numerically that the effective potential of the case (ii) is lower than that of the case (i). In the case (i), $R = R'$ and $T = T'$, combining Eqs. (39) and (40), we have

$$\begin{aligned}\Delta S[\psi,\bar{\psi},R,T] =&\beta\sum_j\Bigg\{\sum_n\left[(R^j_{\alpha\beta})^2+(T^j_{\alpha\beta})^2\right]\\ &-\sum_k\bar{\psi}_k\Big[R^{jT}P_0^+-R^jP_0^-\\ &+i\left(T^{jT}P_0^++T^jP_0^-\right)\Big]\cos k_j\psi_k\Bigg\}.\end{aligned} \tag{A1}$$

Since $\cos k_j$ is even under time-reversal, we may choose such that

$$\begin{cases} R^j = \phi_j\gamma_0 = \phi_j\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}, \\ T^j = -i\omega_j I = -i\omega_j\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \end{cases} \tag{A2}$$

where $\phi_j$, $\omega_j$ are constants. In this case, we see that the correction from the strong coupling limit is equivalent to the modification of the masses of doublers. That is, the effective action is obtained by replacing $\cos k_j$ in $\mathcal{M}(\boldsymbol{k},\sigma)$ (Eq. (34)) by $(1+\beta\phi_j+r\beta\omega_j)\cos k_j$. Then we obtain the effective potential expressed by auxiliary fields:

$$\begin{aligned}\mathcal{F}_{\text{eff}}(\sigma,\phi_j,\omega_j) =& \sigma^2+4\beta\sum_j(\phi_j^2-\omega_j^2)\\ &-\int_{-\pi}^{\pi}\frac{d^3k}{(2\pi)^3}\log\left[\det\mathcal{M}(\boldsymbol{k},\sigma,\phi_j,\omega_j)\right].\end{aligned} \tag{A3}$$

Eliminating $\phi_j$ and $\omega_j$ by the stationary conditions $\partial F_{\text{eff}}(\sigma,\phi_j,\omega_j)/\partial\phi_j = \partial F_{\text{eff}}(\sigma,\phi_j,\omega_j)/\partial\omega_j = 0$, we arrive at the effective potential up to $\mathcal{O}(\beta)$:

$$\begin{aligned}\mathcal{F}_{\text{eff}}(\sigma) =& \sigma^2-2\int_{-\pi}^{\pi}\frac{d^3k}{(2\pi)^3}\log\left[\left(m_{\boldsymbol{k}}-\frac{\sigma}{2}\right)^2+\sum_l\sin^2 k_l\right]\\ &-(1-r^2)\beta\sum_{j=1}^{3}\left[\int_{-\pi}^{\pi}\frac{d^3k}{(2\pi)^3}\frac{\left(m_{\boldsymbol{k}}-\frac{\sigma}{2}\right)\cos k_j}{\left(m_{\boldsymbol{k}}-\frac{\sigma}{2}\right)^2+\sum_l\sin^2 k_l}\right]^2.\end{aligned} \tag{A4}$$

Comparing Eq. (A4) and Eq. (45), we see that the ground state is realized in the case (ii) [see Fig. 3].

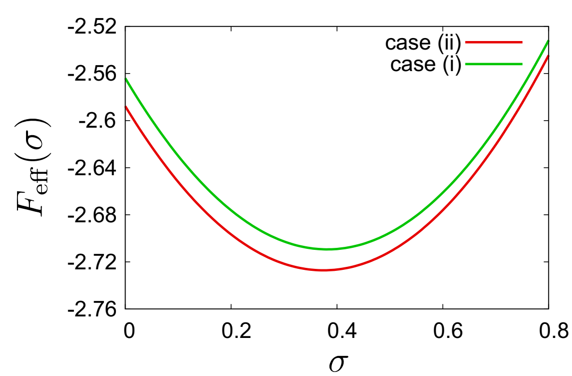


FIG. 3. (Color online) Comparison of $F_{\text{eff}}(\sigma)$ in the case (i) and (ii). $r = 0.50$, $m_0 = -0.50$, $\beta = 0.30$.

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